NEED TO KNOW
a national security newsletter

Volume 1, Number 3 April 2001

Defining Excellence –
Modeling, Simulation and Visualization

Computer science may not at first glance appear to be a national security component. But the Department of Energy recognizes that advanced computing lies at the heart of all technological advancement. A look at the DOE Headquarters National Security Web site confirms this view. Right there with categories of Security, Emergency Response, and Nonproliferation is Computing. And right there is modeling, simulation and visualization.

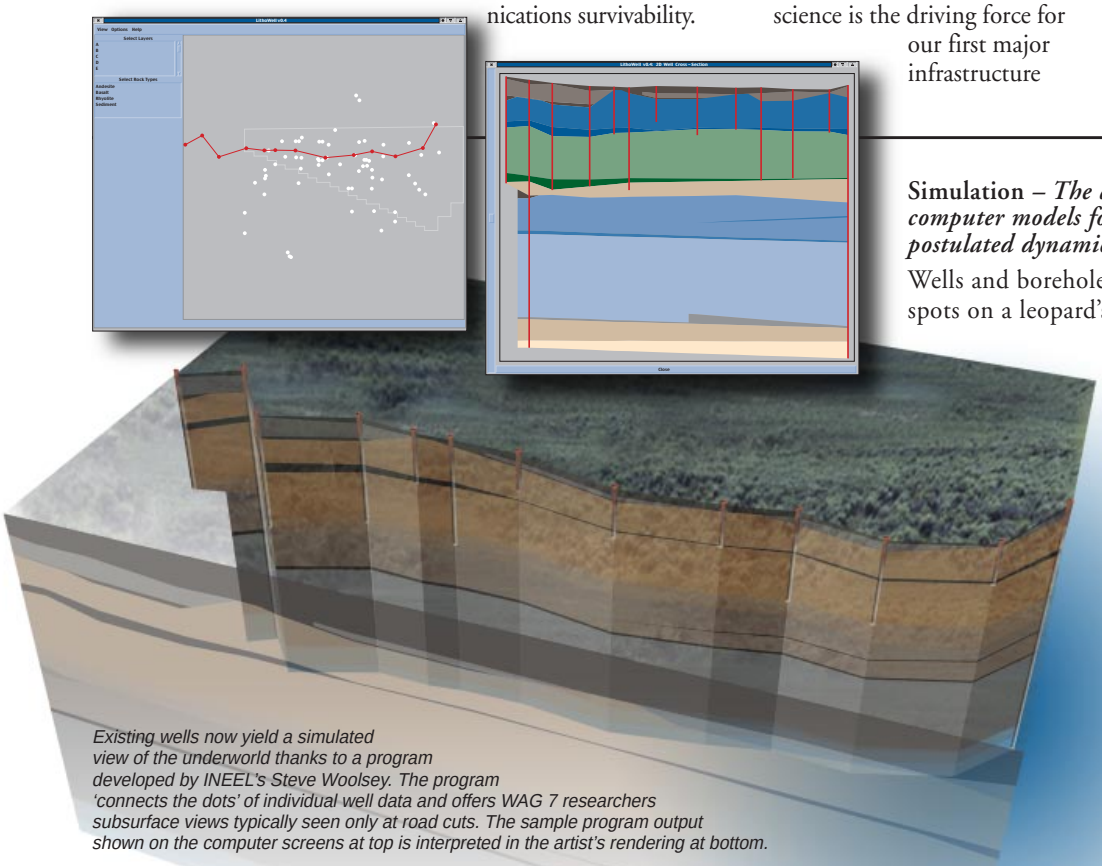
"National security has been ***the*** driving force in many of our country's computational and communication advances," says Jane Gibson, manager of Software and Electronics and the modeling, simulation and visualization group. "In the 1960s, the Defense Advanced Research Projects Agency funded the creation of the Internet to ensure communications survivability.

"Our nation's security mission has historically required the fastest computers available. For example, DOE sponsors the Accelerated Strategic Computing Initiative, which uses terascale computers to simulate nuclear tests instead of conducting them. INEEL, for the first time in a long, long time, is in the position of joining the top 500 club in high-performance computing with its recent acquisition of shared memory computers and improved connectivity to the research world.

"In INEEL's case, subsurface science is the driving force for our first major infrastructure improvements, and all other INEEL institutional plan initiatives have joined forces to leverage these investments to benefit all through the recent adoption of a companywide initiative, 'Advanced Computing and Collaboration Initiative.'"

Gibson says the capabilities of the INEEL's National Security Modeling, Simulation and Visualization are superior. The reputation of key members is world-class and their research and development renowned. They define excellence.

Take a virtual tour of these capabilities through these brief descriptions of some of the organization's projects.



Existing wells now yield a simulated view of the underworld thanks to a program developed by INEEL's Steve Woolsey. The program 'connects the dots' of individual well data and offers WAG 7 researchers subsurface views typically seen only at road cuts. The sample program output shown on the computer screens at top is interpreted in the artist's rendering at bottom.

Simulation – ***The development and use of computer models for the study of actual or postulated dynamic systems.***

Wells and boreholes dot the INEEL landscape like spots on a leopard's hide. Hundreds pierce the thin skin of the high-desert soil, auguring through layers of sediment and basalt. The depths range from the shallow vadose or geotechnical wells at less than 100 feet to the deep geological investigation boreholes sunk nearly 5000 feet into the subsurface.

In addition to performing the task they were drilled to do – supplying water or monitoring the environment – the wells tell the story of the earth beneath them. The wells reveal what

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State of the Division

Laurin Dodd,
Associate Laboratory Director, National Security

On Saturday, March 24, the 179th Airlift Wing of the Air National Guard flew a C-130 into Idaho Falls to pick up the AN/TSQ-209 Communication Central. With careful maneuvering, the –209 was backed into the belly of the plane and flown the next day to its final destination in Illinois.

The January newsletter featured a story on the AN/TSQ-209, the command-and-control system designed by National Security for the Air Force. Just last month, a successful chapter in that program ended when the Air National Guard flew in to pick up a -209 unit to transport it to its final destination in Illinois. I know everyone in the program felt real gratification in seeing a job well done. The program, the INEEL and Idaho should be proud.

Our opportunity to be involved in ASOC and other large engineered systems for the Department of Defense has received strong support over the years from our congressional delegation. This support began with Gov. Dirk Kempthorne while he was a U.S. senator and continues with senators Larry Craig and Mike Crapo and Rep. Mike Simpson. We know that they share this success with us.

This issue includes an article on the portable isotopic neutron spectroscopy system. PINS is a classic example of how a national laboratory can and should develop and deploy new technology. PINS was invented here, won an R&D 100 award in 1992 and has since been deployed around the world. This technology has been a cornerstone of our major engineered systems including MMAS, TMAS and Pine Bluff Arsenal.

We continue to recognize the achievements and contributions of National Security employees in this newsletter. Individually and as a team, these efforts ensure the success of our mission.

COMPUTING *(continued from page 1)*

rock types, at what depths lay in their path downward. Until recently, this information was more isolated, and difficult and time-consuming to combine. But no longer. Steve Woolsey has developed a subsurface lithographic model that easily 'connects the dots' of the individual wells, offering a simulated view of the underworld.

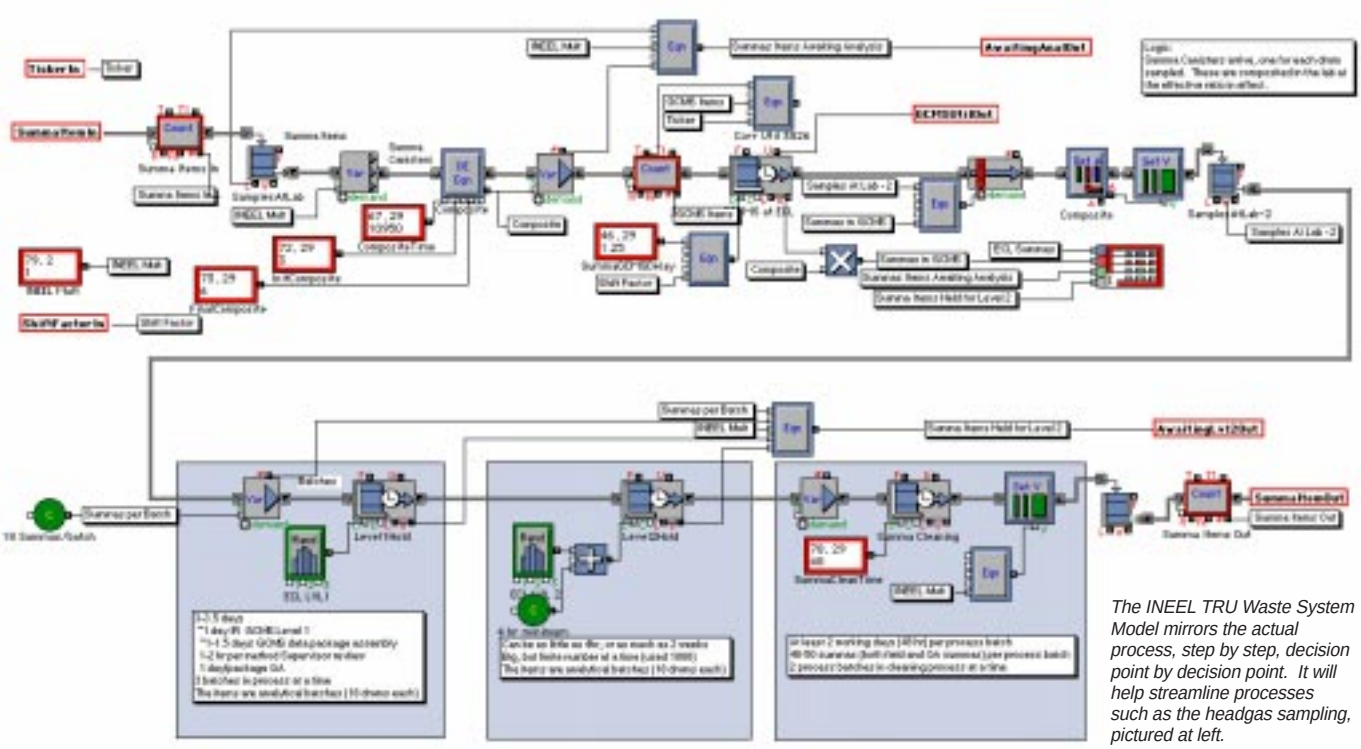
Woolsey's program peels back the skin of the Site and shows subsurface views of the INEEL typically seen only at road cuts or within open mines. Developed for Waste Area Group 7 at the Radioactive Waste Management Complex, INEEL scientists researching the migration of contaminants through the labyrinth of rock, soil and water now have another tool.

The program started with a database containing the facts on each well – the types of soil and rock it drilled through and depths of each stratum. The database can be queried for each well. Woolsey added a "rule set" developed by Steve Anderson, a geologist with the United States Geological Survey. The "rule set" suggested logical guidelines for interpreting geological connections between two wells.

On a computer screen, INEEL wells are displayed on a map, and with a click of a mouse, Woolsey selects wells and connects them in a line. Using complex algorithms, the program interprets the individual well data and displays a view that Woolsey says, "looks like the side of a mountain where an earthquake fault has risen and revealed the layers of earth." WAG 7 researchers can now visualize the surface beneath the INEEL and its complex layering of rock.

Woolsey's next step will be tying in the code for associate James Galbraith's visualization work with contaminant data. While developed specifically to address WAG 7 concerns, the program will be evaluated for site-wide use.

– Steven Woolsey, woolsr@inel.gov



The INEEL TRU Waste System Model mirrors the actual process, step by step, decision point by decision point. It will help streamline processes such as the headgas sampling, pictured at left.

Modeling – ***A mathematical or physical system, obeying certain specified conditions, whose behavior is used to understand a physical, biological or social system to which it is analogous in some way.***

The INEEL committed to removing 3,100 cubic meters of transuranic waste from Idaho by December 31, 2002. To accomplish this, over 24,000 contact-handled 55-gallon drums will be examined at the Stored Waste Examination Pilot Plant to yield the 15,000 shippable drums. All of the drums undergo various processes including real-time radiography, gamma-ray spectrometry, venting, and headspace gas sampling before loading and shipping. Selected drums will also go through intrusive examination and sampling.

An onerous task at best, delays in opening the Waste Isolation Pilot Plant and changes to the waste acceptance criteria compressed the INEEL's performance time down to 27 months.

To ramp up for this massive production effort, the existing process had to undergo changes – but what changes? The right changes could increase productivity; the wrong ones could cause unacceptable delays.

That's where Dave Van Haaften came in. Van Haaften and Modeling, Simulation and Visualization supervisor Cathy Barnard created a system model of the complete INEEL TRU waste project.

Based on a national model they developed for the Carlsbad Field Office, the INEEL TRU Waste System Model mirrors the actual process, step by step, decision point by decision point. The model was developed in Extend, a commercial discrete event simulation software package. The INEEL model simulates events that happen when items - in this case drums – move through the process.

Built into the system are the time delays – how long each operation delays a drum at any given point in the process. The delay data was developed from design files, project manager input and interviews with operators. The model shows the bottlenecks in the process.

The purpose of the model was to guide and validate planning and it has done that, demonstrating the need for additional capacity in several areas including real-time radiography. As a result, the first rental RTR began operating in April. A second 7 x 12 shift was based, in part, on the model's results.

Industrial manufacturers have long depended on discrete event models; 3100m^3 is one of the first 'production' projects on Site to develop one. The ability to view different scenarios before implementation of process changes has proven to be invaluable.

– Dave Van Haaften
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Scaling – ***Expressing the terms in an equation of motion in powers of nondimensional quantities (such as a Reynolds number), so that terms of significant magnitude under conditions specified in the problem can be identified, and terms of insignificant magnitude can be dropped.***

The INEEL has long been a center of excellence for use of scaling in research and development. And no better example exists than the Semiscale facility, constructed at the Water Reactor Research Test Facility in the early '70s. Roughly 1/1700th the size of a power reactor, this scaled-down version was built to help understand what happens in a massive loss of coolant accident (LOCA).

Tom Larson, engineer and science fellow explained the concepts of scaling, Semiscale experiments, and some of the results. "Scaling culminates with the art of building a small system representing a larger system so that the first order of effects are preserved and the lower order effects are maintained as much as possible." Different size reactors, pipes and systems do not respond exactly the same; the art is recognizing the distortions and their effects.

"We were tasked to show if (power) plants could survive the worst case accidents. We experimented with double breaks in cooling pipes to provide data that could be used to help develop and assess the computer models." In some early experiments, the researchers put food coloring in the water to check where the cooling water went in an accident. The phrase "all the green water went on the floor" wasn't good but the experiments at Semiscale were and caused the Atomic Energy Commission to adopt more conservative licensing and operating requirements.

Larson adds, "Interestingly, the accident at Three Mile Island was a result of small break loss of coolant, not the large break LOCAs conducted at Semiscale. Luckily, the Loss Of Fluid Test facility at the Test Area North as well as the Semiscale facility could be modified and used and did conduct a series of small break LOCA experiments."

Nowadays Larson is involved with many scaling projects ranging from developing a nonintrusive flow device for Advanced Test Reactor applications to measuring the flow rate of cold air entering and warm air exiting manufactured homes. He has spent the last several months building support and establishing the groundwork for the new lab-wide computing initiative. But Larson is looking forward to the challenge of subsurface fate and transport research.

"Reactor scaling had enough nonlinearity but at least as far as we know, it is primarily a single scale problem. Subsurface fate and transport is a multi-scale problem. Fluid-flow, radiation, porosity, biological effects, etcetera, all have to be considered. And there are extremes of scale – geological time scale covers epochs, other temporal scales will be much smaller and multiple physical scales exist. From a scaling viewpoint, researchers know they have a problem, they just don't know the magnitude."

– Tom Larson
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Artificial Intelligence – ***The property of a machine capable of reason by which it can learn functions normally associated with human intelligence.***

Gail Cordes doesn't care for the popular term 'artificial intelligence.' She prefers the more accurate 'intelligent information processing' or 'computational intelligence.' Whatever the term used, it is the extraordinary concept of increasing computer efficiency by mimicking ways the human brain processes information.

Cordes has been involved with intelligent information processing since 1988 and describes it then as a "bootstrap operation." The program has gone far in the intervening years. She explained some of the applications that cross-organizational teams have developed at the INEEL.

Expert systems – computer systems composed of algorithms that execute specialized, usually difficult professional tasks – are designed to perform at the level of or even beyond the level of a human expert. Expert systems follow a series of logic steps,

Roughly 1/1700th the size of a power reactor, the Semiscale facility was built to help understand what happens in a massive loss of coolant accident (left).

A data review expert system is employed in the passive/active neutron and gamma assay conducted at SWEPP. The expert system flags discrepancies for a human to review (right).

with each path defined by a 'yes-no' response.

Back in '88, Cordes was the project manager for the Nuclear Regulatory Commission's Reactor Safety Assessment System. This expert system used plant data to assess the safety status of a commercial nuclear power reactor experiencing a long-term disturbance. More recently, a team of researchers from Waste Management Technologies has developed a data review expert system that is employed in the passive/active neutron and gamma assay conducted at the Stored Waste Examination Pilot Plant on the INEEL. The system analyzes data on the waste drums and flags discrepancies for a human to review.

Fuzzy logic is called the logic of approximate reasoning and deals with uncertainties. It allows for interpretation and 'decision-making' by computers and is now so accepted that common household appliances are advertised as having it. "Powerful but surprisingly simple" Cordes describes it. In one of Cordes' early successes using this tool, she and two colleagues from Industrial and Material Technologies demonstrated a fuzzy control system for the Cybertran, the electronic train developed at the INEEL.

Cordes' current projects are also team efforts, supported by funding and direction from programs outside of National Security. One project, through Waste Management Technologies, employs pattern recognition to monitor the performance of nondestructive assay technologies. NDA technologies are used to characterize materials and container contents and the resulting characterization information becomes an historic, archival record. The software program uses the patterns of historic operation data to evaluate the ongoing equipment operation, providing real-time capability to monitor and defend performance. This software is also being used to interpret the NDA characterization measurement data.

A layperson may call these techniques artificial intelligence but Cordes says that by whatever name you use, it can assist humans in everything from safely running a nuclear reactor to more accurately interpreting X-rays.

– Gail Cordes
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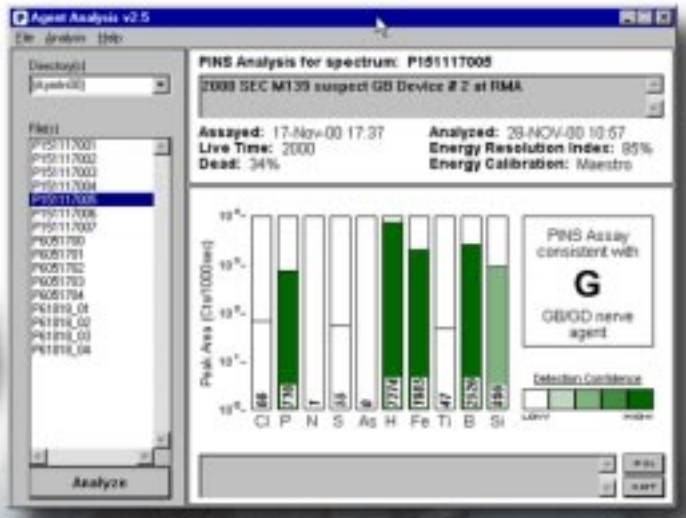
CONTINUED NEXT ISSUE…

INEEL Technology Used at Rocky Mountain Arsenal

Arsenal Bomblets Identified with Pins



One of the softball-sized bomblets discovered at Rocky Mountain Arsenal (above). The INEEL's PINS device safely analyzes a bomblet's contents (right). An example analysis screen from the PINS technology reveals the bomblet's contents to be sarin, a deadly nerve gas (above right).

The discovery of six softball-sized chemical warfare munitions at Rocky Mountain Arsenal just outside of Denver made headlines across the nation. What didn't make the news is that an INEEL technology, the portable isotopic neutron spectroscopy system, was used to confirm the contents of the "bomblets" as the nerve agent sarin.

The INEEL system, PINS, nonintrusively identifies material within steel and other containers using gamma spectroscopy. Using a radioisotopic source, PINS shoots a beam of neutrons through the metal of a container. The neutrons interact with the elements inside and produce high-energy gamma rays.

The gamma rays passing back out are detected by a spectrometer. As distinctive as fingerprints, every chemical emits its own signature gamma rays. The software within PINS analyzes the gamma ray spectra and identifies the fill.

The U.S. Army acquired PINS seven years ago and regularly conducts analyses of chemical weapons to confirm their content. The military is in the process of destroying Cold War stockpiles under the provisions of the Chemical Weapon Convention.

But there is a difference between obsolete, stockpiled weapons and recently discovered, rusty, half-buried bombs. Often these munitions have lost their identification markings due to corrosion and exposure to the elements.

So in the case of "nonstockpile" chemical weapons, the Army conducts a multi-disciplinary assessment to identify the contents. Experts in radiography, explosive ordnance disposal, chemical warfare agent chemistry and Army chemical weapons history, along with a member of the INEEL PINS team, assess the evidence and determine the munitions' chemical fill.

"The Army is very careful," says Gus Caffrey, PINS developer and INEEL nuclear physicist. "The consequences of an accident are severe and could include a fatality. So INEEL scientists review spectra from all suspect nonstockpile chemical munitions and containers."

Caffrey happened to be back east when the first Rocky Mountain Arsenal bomblet was discovered and assessed with X-rays and PINS. The Army e-mailed the spectra to the INEEL, where Brian Harlow and Ken Krebs of the PINS team interpreted them. Harlow and Krebs forwarded their analysis to Caffrey in Edgewood, Md., for a meeting with the Army's assessment team. Edgewood is headquarters to the Soldiers, Biological, and Chemical Command and its Technical Escort Unit. These are the soldiers who are trained to respond to this type of emergency.

Caffrey agreed with the analysis. "The bomblets' gamma spectra aren't subtle," says Caffrey. "The phosphorus and hydrogen peaks clearly indicated a sarin fill."

That was the first of six confirmed sarin-filled spheres. Sarin was first developed in Germany, prior to World War II. It was named for the developers, **S**chrader, **A**mbrose, **R**udriger and van der **Lin**de. Sarin is a very toxic nerve agent that is fatal either inhaled as a vapor or absorbed through the skin; as little as a gram can kill an adult. Sarin is also known by its NATO designation, agent GB.

In February, the Army began detonating the bomblets in a steel chamber shaped somewhat like a home-sized concrete mixer. The sarin is then neutralized with a caustic solution that renders it safe, preventing environmental contamination or health threats.

PINS, without headlines and without fanfare, helped diffuse a potentially deadly situation.

– Gus Caffrey
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Achievements, Accomplishments and Acknowledgements

The Transuranic Reporting, Inventory and Processing System (TRIPS) digital signature process won a 2001 Pollution Prevention Award from the Department of Energy Headquarters. The patent-pending technology was recognized for eliminating stacks of paper while maintaining data integrity. The award submission included the entire TRIPS team with Wayne Austad as point-of-contact. A new book titled *PKI [Public Key Infrstructure]: A Wiley Tech Brief*, by Tom Austin was published in December and Chapter 16 is a case study of the TRIPS digital signature system written by Austad. Reviews of the book have been very favorable. Idaho Falls television station KIFI Channel 8, interviewed Austad and engineer Sheila Hailey for an informative and positive profile of the technology aired in late March.

- Keith Daum received notice that "Formation of Halide Reactant Ions in Ion Mobility Spectrometry and Effects on the Ionization and Detection of TNT" has been accepted for publication in *Talanta*. Daum submitted another article, "The Role of Oxygen in the Formation of TNT Product Ions in Ion Mobility Spectrometry" to the *International Journal of Mass Spectrometry*. Daum completed and defended his Ph.D. dissertation, "Selective Ion-Molecule Chemistry to Enhance Detection in Ion Mobility Spectrometry," at the University of Idaho. This dissertation comprised the above articles on making TNT analysis more reliable.
- On March 13, Terry Creque successfully defended his dissertation, completing the last of the requirements for his Ph.D. in biology. Creque will receive his degree from George Mason University in June. Creque is currently assigned to the Department of Energy, Office of Defense Nuclear Nonproliferation in the Chemical and Biological National Security Program in Washington D.C.
- Dennis Bingham was honored at the 5th Annual Inventors Recognition Banquet. The award was for the patent, "Apparatus and Process for the Refrigeration, Liquefaction, and Separation of Gases with Varying Levels of Purity."
- John Jenkins successfully completed the first section of the Toastmaster International Communication and Leadership Program.
- Lynn Dean was recognized by the Project Leaders for Stage II of the Operable Unit 7-10 Staged Interim Action Project for his outstanding contribution to the project. "Lynn's hard work, expertise, continued professionalism, and exceptionally logical thought processes had a major impact on the clarity and acceptance of the DAMS (Data Acquisition and Management System) design delivered to the Agencies."
- The PINS Team was recognized for their support in the assessment of the Rocky Mountain Arsenal bomblets by William Brankowitz, deputy to the PM/Non-Stockpile, a unit of PM/Chem Demilitarization at Edgewood, Md. (See full story on page xx) "Congratulations to the EDS (emergency destruct system) team on the successful detonation of the sixth and final bomblet… at RMA. Senator Allard is enroute to present the organizational award to PMCD… Again, congratulations on a job well done."
- John Morrison, Michael Fryer and Andrea Vail received a patent on "Method and Apparatus for Measuring Butterfat and Protein Content Using Microwave Absorption Techniques."
- Lyle Roybal received a patent on "Method for Detecting the Presence of a Ferromagnetic Object."
- Dennis Bingham, Richard Swainston, Gary Palmer and Russell Ferguson received a patent on "Methods and Apparatuses for Cutting, Abrading and Drilling."
- Brett Rasmussen, Catherine Herring, and Wayne Austad filed a provisional patent for "Digital Signing of HTML Forms."

Counterintelligence Corner

Employees often assume Counterintelligence to be an arm of Security. On the contrary, it is an intelligence function whose primary purpose is to stop the international theft of United States technology. Targets for espionage activities are often the Laboratory's scientists and researchers. "What better way to offer support and guidance to those very individuals than to be part of the R&D organization," says Jack Way, Counterintelligence Program manager.

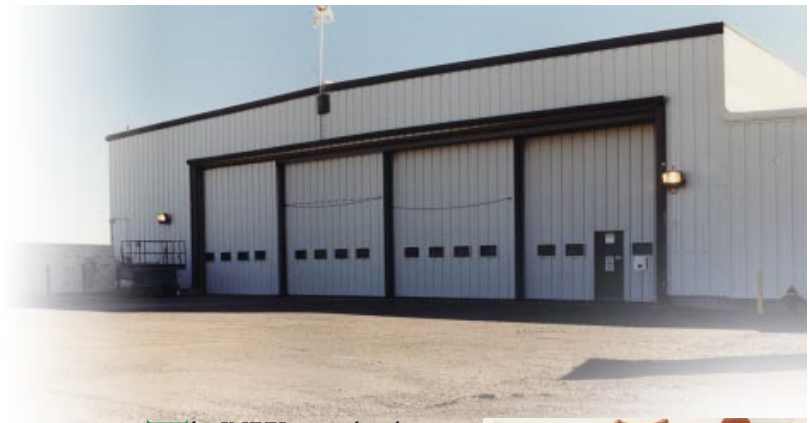
Way's explanation is a prelude to a new, regular feature to be included in the National Security Division's *Need to Know.*

Purpose of the feature is to continue to "get the word out," explain program components, emphasize the reality of the threat and to publicize services offered. The feature will announce Department of Energy CI program updates and alert employees to issues.

Upcoming topics include specific threats to the INEEL including computer threats, targeted technologies, risk to travelers, the insider threat and the polygraph program.

Look for more information to appear in the next quarterly issue. In the meantime, explore the Counterintelligence Program **internal** Web site.

Material Science Support Laboratory



The Material Science Support Laboratory almost triples the secure laboratory space available for the National Security Division. Installation of specialized equipment continues in each of the four laboratory bays, including a robot arm for the plasma spray unit (top right), a hot press (above right), and a vacuum spray booth (above left).

The INEEL completed renovation of a facility for materials science research and the National Security Division began operations in late March. At 8400 square feet, the Material Science Support Laboratory almost triples the secure laboratory space available for the Division. Located at the Central Facilities Area, the MSSL was constructed from the vacant security helicopter hangar adjacent to the existing Security Headquarters. In addition to the laboratory bays, the renovated facility includes a classified conference room that will be available to multiple programs.

"This may be the only secure laboratory facility in the DOE Complex with a rapid response security force in the next room," said Doug Hall, MSSL project manager for National Security.

The INEEL has an illustrious history in materials science, dating from its earliest days in reactor design and testing when the burgeoning nuclear industry needed new materials to withstand sustained reactions. This research and subsequent development evolved into significant ongoing materials programs at the Laboratory, such as the protective armor manufactured for the U.S. Army Abrams tanks by the Specific Manufacturing Capability Project, located at Test Area North.

Materials research conducted at MSSL will support other INEEL programs in addition to those of National Security.

Some of the first research to take advantage of the new facility are projects related to the behavior of energetic materials and production of lightweight armor composites.

Originally constructed in 1984, the hangar served different operational purposes for several years after the retirement of the security helicopter. However, its relatively new condition and high-bay access made it the ideal candidate when the need for secure laboratory space became paramount. Another factor compounding the need for space was the acquisition of specialized plasma spray equipment from the closing DOE Mound facility in Miamisburg, Ohio. The equipment was too large for installation in existing laboratories. Once operational, this equipment will add unique capabilities to the Laboratory's ongoing plasma spray research.

"The design, construction and operation of the MSSL is a tribute to the cooperative efforts of R&D and Operations Branch personnel," Laurin Dodd, Associate Laboratory Director for National Security, said while discussing the joint efforts to plan and build the multi-program laboratory.

The INEEL will have invested approximately $1.5 million into the upgrades. Research work generated by the laboratory over the next five years has the potential of returning that investment many times.

NEED TO KNOW *is a publication of the National Security Division of the Idaho National Engineering and Environmental Laboratory. The INEEL is a science-based, applied engineering national laboratory dedicated to supporting the U.S. Department of Energy's missions in environment, energy, science and national security. The INEEL is operated for the DOE by Bechtel BWXT Idaho, LLC, in partnership with the Inland Northwest Research Alliance. Requests for additional copies, story ideas or questions should be directed to the editor at (208) 526-1058, kzc@inel.gov. This is printed on recycled paper.*

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